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EFFECTS OF LONG-RANGE DISPERSION IN NONLINEAR DYNAMICS OF DNA MOLECULES

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A discrete nonlinear Schrödinger (NLS) model with long-range dispersive interactions describing the dynamical structure of DNA is proposed. Dispersive interactions of two types: the power dependence r^{-s} and the exponential dependence $e^{-\beta r}$ on the distance, r, are studied. For s less than some critical value, s_{cr}, and similarly for $\beta \leq \beta_{cr}$ there is an interval of bistability where two stable stationary states : narrow, pinned states and broad, mobile states exist at each value of the total energy. For cubic nonlinearity the bistability of the solitons occurs for dipole-dipole dispersive interaction ($s = 3$), and for the inverse radius of the dispersive interaction $\beta \leq \beta_{cr} = 1.67$. For increasing degree of nonlinearity, σ, the critical values s_{cr} and β_{cr} increase. The long-distance behavior of the intrinsically localized states depends on s. For $s > 3$ their tails are exponential while for $2 < s < 3$ they are algebraic. A controlled switching between pinned and mobile states is demonstrated applying a spatially symmetric perturbation in the form of a parametric kick. The mechanism could be important for controlling energy storage and transport in DNA molecules.

1 Introduction

Understanding the mechanisms of the functioning of biological macromolecules (proteins, DNA, RNA, etc.) remains for now the major challenge in molecular biology. One of the most important questions is the understanding of gene expression. The expression of a given gene involves two steps: transcription and translation. The transcription includes copying the linear genetic information into the messenger ribonucleic acid (mRNA). The information stored in mRNA is transferred into a sequence of aminoacids using the genetic code. mRNA is produced by the enzyme RNA-polymerase (RNAP) which binds to the promoter segment of DNA. As a result of the interaction between RNAP and promoter of DNA the so-called "bubble" (i.e. a state in which 10–20 base pairs are disrupted) is formed. The disruption of 20 base pairs corresponds to investing some 100 kcal/mole (0.43 eV) [1].

In the framework of a linear model the large-amplitude motion of the bases was supposed to occur due to an interference mechanism [2]. According to this model energetic solvent molecules kick DNA and create elastic waves therein. As a result of the interference of two counter propagating elastic waves, the base displacements may exceed the elasticity threshold such that DNA undergoes a transition to a kink form which is more flexible. A similar approach was also proposed [3,4]. The linear elastic waves in DNA are assumed to be strong enough to break a hydrogen bond and thereby facilitate the disruption of base pairs. In spite of the attractiveness of this theory which gives at least a qualitative interpretation of the experimental data [5] there are following fundamental difficulties which to our opinion are inherent to the linear model of the DNA dynamics: i) The dispersive properties (the dependence of the group velocity on the wave-length) of the vibrational degrees of freedom in DNA will cause spreading of the wave packets and therefore smear the interference pattern. Furthermore, it has been shown [6] that the amplitudes of the sugar and the base vibrations are rather large even in a crystalline phase of DNA. Since the large-amplitude vibrations in the molecules and the molecular complexes are usually highly anharmonic their nonlinear properties can not be ignored. ii) Molecules and ions which exist in the solution permanently interact with DNA. These interactions are usually considered as white noise and their influence is modelled by introducing Langevin stochastic forces into the equations describing the intramolecular motion. It is well known [7] that stochastic forces provide relaxation of linear excitations and destroy their coherent properties. Equivalently the coherence length (the length of the concerted motions) rapidly decreases with increasing temperature. iii) DNA is a complex system which has many nearly isoenergetic ground states and may therefore be considered as a fluctuating aperiodic system. DNA may have physical characteristics in common with quasi-one-dimensional disordered crystals or glasses. However, it is known [8] that the transmission coefficient for a linear wave propagating in disordered chain decreases exponentially with the growth of the distance (Anderson localization). In this way it is difficult to explain in the framework of linear theory such a phenomenon as an action at distance where concerted motion initiated at one end of a biological molecule can be transmitted to its other end.

The above mentioned fundamental problems can be overcome in the framework of nonlinear models of DNA. Nonlinear interactions can give rise to very stable excitations, called solitons, which can travel without being smeared out. These excitations are very robust and important in the coherent transfer of energy [9]. For realistic interatomic potentials the solitary waves are compressive and supersonic. They propagate without energy loss, and their collisions

are almost elastic.

Nonlinear interactions between atoms in DNA can give rise to intrinsically localized breather-like vibration modes [10,11]. Localized modes being large-amplitude vibrations of a few (2 or 3) particles, can facilitate the disruption of base pairs and in this way initiate conformational transitions in DNA. These modes can occur as a result of modulational instability of continuum-like nonlinear modes [12] which is created by energy exchange mechanisms between the nonlinear excitations. The latter favors the growth of the large excitations [13].

Nonlinear solitary excitations can maintain their overall shape on long time scales even in the presence of the thermal fluctuations. Their robust character under the influence of white noise was demonstrated [14] and a simplified model of double-stranded DNA was proposed and explored. Quite recently the stability of highly localized, breather-like, excitations in discrete nonlinear lattices under the influence of thermal fluctuations was investigated [15]. It was shown that the lifetime of a breather increases with increasing nonlinearity and in this way these intrinsically localized modes may provide an excitation energy storage even at room temperatures where the environment is seriously fluctuating.

Several theoretical models have been proposed in the study of the nonlinear dynamics and statistical mechanics of DNA (see the very comprehensive review [16]). A particularly fruitful model was proposed by Peyrard and Bishop [17] and Techera, Daemen and Prohofsky [18]. In the framework of this model the DNA molecule is considered to consist of two chains that are transversely coupled. Each chain models one of the two polynucleotide strands of the DNA molecule. A base is considered to be rigid body connected with its opposite partner through the hydrogen-bond potential $V(u_n)$, where u_n is the stretching of the bond connecting the bases, n, and $n = 0, \pm 1, \pm 2, ..$ is labelling the base-pairs. The stretching of the n'th base-pair is coupled with the stretching of the m'th base-pair through a dispersive potential $K(u_n, u_m)$. The process of DNA denaturation was studied [17,19] under the assumption that the coupling between neighboring base-pairs is harmonic $K(u_n, u_{n+1})$. An entropy-driven denaturation was investigated [20] taking into account a nonlinear potential $K(u_n, u_{n+1})$ between neighboring base-pairs. The Morse potential was chosen [17,19,20] as the on-site potential $V(u_n)$ but also the longitudinal wave propagation and the denaturation of DNA has been investigated [14] using the Lennard-Jones potential to describe the hydrogen bonds.

In the main part of the previous studies the dispersive interaction K was assumed to be short-ranged and a nearest-neighbor approximation was used. It is worth noticing, however, that one of two hydrogen bonds which is responsible for the interbase coupling: the hydrogen bond in the $N - H...O$ group is characterized by a finite dipole moment. Therefore a stretching of

the base-pair will cause a change of the dipole moment so that the excitation transfer in the molecule will be due to transition dipole-dipole interaction with a $1/r^3$ dependence on the distance, r. It is also well known that nucleotides in DNA are connected by hydrogen-bonded water filaments [21,22]. In this case an effective long-range excitation transfer may occur due to the nucleotide-water coupling.

In the last few years the importance of the effect of long-range interactions (LRI) on the properties of nonlinear excitations was demonstrated in several different areas of physics. The effective mass of solitons in the Frenkel-Kontorova model with a repulsive LRI, their shapes and Peierls barriers were investigated [23]. An implicit form of solitons was obtained [24] in a sine-Gordon system with a LRI of the Kac-Baker type [25,26] and the dependence of the soliton width and energy on the radius of the LRI was analyzed. It was postulated [27] that the nonlinear term in the sine-Gordon equation has a non-local character and novel soliton states, of topological charge zero, were found to exist at a large enough radius of the interaction. The effects of long-range interactions of the Kac-Baker type were studied in static and dynamic nonlinear Klein-Gordon models [28], and nonlinear Schrödinger [29] continuum models. The effects of a long-range harmonic interaction in a chain with short-range anharmonicity were also considered [30]. It was demonstrated that the existence of two velocity dependent competing length scales leads to two types of solitons with characteristically different widths and shapes for two velocity regions separated by a gap. A nonlocal NLS equation was proposed [29] for systems with long-range dispersion effects. In contrast to the usual NLS equation stationary solutions only exist for a finite interval of the number of excitations. In the upper part of this interval two different kinds of stationary solutions were found. The new one containing a cusp soliton was shown to be unstable. It was also pointed out that moving solitons radiate with a wavelength proportional to the velocity. Quite recently [31] we proposed a new nonlocal discrete NLS model with a power dependence on the distance of matrix element of dispersive interaction. It was found that there is an interval of bistability in the NLS models with a long-range dispersive interaction. One of these states is a continuum-like soliton and the other is an intrinsically localized mode.

The goal of this contribution is to investigate the effects of long-range interactions on the nonlinear dynamics of the two-strand model of DNA. In Sec. II we present the analytical theory and the results of numerical simulations of stationary states of the discrete NLS model with a long-range dispersive interaction. We discuss the bistability phenomenon for the soliton solutions and their stability. In the analytical part of this section we use a variational approach exploiting an exp-like function as a trial function. Then, in Sec. III

we investigate the long-distance behavior of the nonlinear excitations and show that intrinsically localized states of the discrete NLS model with a dispersive interaction decaying slower than $1/r^3$ have algebraic tails. Section IV is devoted to the investigation of switching between bistable states. We show that a controlled switching between narrow, pinned states and broad, mobile states with only small radiative losses is possible when the stationary states possess an internal breathing mode.

2 System and equations of motion

We study the two-strand model of DNA which is described by the Lagrangian

$$L = T - K - V \ , \tag{1}$$

where

$$T = \frac{1}{2} \sum_n \left(\frac{d\, u_n}{d\, t} \right)^2 \tag{2}$$

is the kinetic energy (the mass of the base-pair is chosen equal to 1),

$$K = \frac{1}{4} \sum_n \sum_{m(n \neq m)} J_{n-m} (u_m - u_n)^2 \tag{3}$$

is the dispersive interbase-pair interaction of the stretchings and

$$V = \sum_n V(u_n) \tag{4}$$

is the potential energy which describes an intrabase-pair interaction. In Eqs. (1)–(4) n and m are site (base-pair) indices, u_n is the base-pair stretching. The value $u_n = 0$ corresponds to the minimum of the intrabase-pair potential $V(u_n)$. We investigate the model with the following power dependence on the distance of the matrix element of the base elastic coupling

$$J_{n-m} = J/|n-m|^s. \tag{5}$$

The constant J characterizes the strength of the coupling. The parameter s is introduced to cover different physical situations including the nearest-neighbor approximation ($s = \infty$), quadrupole-quadrupole ($s = 5$) and dipole-dipole ($s = 3$) interactions. We shall show that this equation having "tunable" properties illuminates both the competition between nonlinearity and dispersion and the interplay of long-range interactions and lattice discreteness. To take

into account the possibility of an indirect coupling between base-pairs (e.g. via water filaments) we consider also the case when the matrix element of the base elastic coupling has the form

$$J_{n-m} = J\, e^{-\beta|n-m|}\ , \tag{6}$$

where β is the inverse radius of the interaction.

Assuming that

$$\left.\frac{\partial^2 V(u_n)}{\partial u_n^2}\right|_{u_n=0} \gg \left.\frac{\partial^j V(u_n)}{\partial u_n^j}\right|_{u_n=0} \qquad \text{for} \quad j=3,4... \tag{7}$$

i.e. the anharmonicity of the intrabase-pair potential is small, we will use a rotating-wave approximation

$$u_n = \psi_n\, e^{-i\omega\, t} + c.c.\ , \tag{8}$$

where $\omega = \sqrt{\left.\frac{\partial^2 V(u_n)}{\partial u_n^2}\right|_{u_n=0}}$ is the frequency of the harmonic oscillations, $\psi_n(t)$ is the complex amplitude which is supposed to vary slowly with time. Inserting Eq. (8) into Eqs. (1)–(4) and averaging with respect to the fast oscillations of the frequency ω we conclude that the effective Lagrangian of the system can be represented in the form

$$\mathcal{L} = \frac{i}{2}\sum_n \left(\dot{\psi}_n\psi_n^* - \dot{\psi}_n^*\psi_n\right) - \mathcal{H}\ . \tag{9}$$

Here $\dot{\psi}_n \equiv \frac{d}{d\tau}\,\psi_n$, $\tau = \frac{t}{2\omega}$.

$$\mathcal{H} = \mathcal{K} + \mathcal{V} \tag{10}$$

is the effective Hamiltonian of the system where

$$\mathcal{K} = \frac{1}{2}\sum_{n,m(n\neq m)}\sum J_{n-m}|\psi_m - \psi_n|^2 \tag{11}$$

is the effective dispersive energy of the excitation and

$$\mathcal{V} = \sum_n \left(\frac{\omega}{2\pi}\int\limits_0^{\frac{2\pi}{\omega}} dt V(\psi_n\, e^{-i\omega\, t} + c.c) - \omega^2\,|\psi_n|^2\right) \tag{12}$$

is the effective intrabase-pair potential. Usually either a Morse potential [17,19] or a Lennard-Jones potential [14] is used to model the hydrogen bonds. With

these potentials however it is very complicated to obtain any analytical results. Therefore to gain insight into the problem we will use a simplified nonlinear potential in the form

$$\mathcal{V} = -\frac{1}{(\sigma+1)} \sum_n |\psi_n|^{2(\sigma+1)} \ , \tag{13}$$

where the degree of nonlinearity σ is a parameter which we include to have the possibility to tune the nonlinearity as well.

From the Hamiltonian (10) we obtain the equation of motion $i\dot{\psi_n} = \dfrac{\partial \mathcal{H}}{\partial \psi_n^*}$ for the wave function $\psi_n(\tau)$ in the form

$$i\dot{\psi_n} + \sum_{m(m\neq n)} J_{n-m}(\psi_m - \psi_n) + |\psi_n|^{2\sigma}\psi_n = 0 \ . \tag{14}$$

The Hamiltonian $\mathcal{H}$ and the number of excitations

$$N = \sum_n |\psi_n|^2 \tag{15}$$

are conserved quantities.

We are interested in stationary solutions of Eq. (14) of the form

$$\psi_n = \phi_n \exp(i\Lambda\tau) \tag{16}$$

with a real shape function ϕ_n and frequency Λ. This reduces the governing equation for ϕ_n to

$$\Lambda\phi_n = J \sum_{m(m\neq n)} |n-m|^{-s}(\phi_m - \phi_n) + \phi_n^{(2\sigma+1)}. \tag{17}$$

Thus Eq. (17) is the Euler-Lagrange equation for the problem of extremizing $\mathcal{H}$ under the constraint $N = constant$.

To develop a variational approach to the problem we use an ansatz for a localized state in the form

$$\phi_n = \sqrt{N \tanh\alpha}\exp(-\alpha|n|) \ , \tag{18}$$

where α is a trial parameter. The ansatz (18) is chosen to satisfy automatically the normalization condition (15) such that the problem of extremizing $\mathcal{H}$ under the constraint $N = constant$ is reduced to the problem of satisfying the equation $\dfrac{d\mathcal{H}}{d\alpha} = 0$.

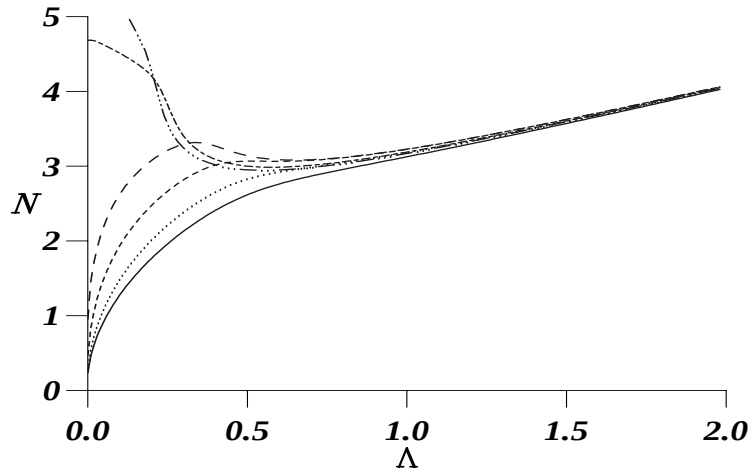

Figure 1: Number of excitations, N, versus frequency, Λ, numerically from Eq. (17) for $s = \infty$ (full), 4 (dotted), 3 (short-dashed), 2.5 (long-dashed), 2 (short-long-dashed), 1.9 (dashed-dotted).

Inserting the trial function (18) into the Hamiltonian given by Eqs. (10), (11), (13) and (5), and evaluating the discrete sums which enter in these equations (see [31] for details) we get the dispersive part of the Hamiltonian

$$\mathcal{K} = 2NJ\left\{\zeta(s) - \tanh(\alpha)F(e^{-\alpha}, s-1) - F(e^{-\alpha}, s)\right\} \tag{19}$$

and the intrabase-pair potential

$$\mathcal{V} = -\frac{N^{\sigma+1}}{\sigma+1}\, f_\sigma \ , \quad \text{with} \quad f_\sigma = \tanh^{\sigma+1}[\alpha]\, \coth[(\sigma+1)\alpha] \ . \tag{20}$$

In Eq. (19)

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} \tag{21}$$

is the Riemann's zeta function and

$$F(z,s) = \sum_{n=1}^{\infty} (z^n/n^s) \tag{22}$$

is the so-called Jonqière's function [32].

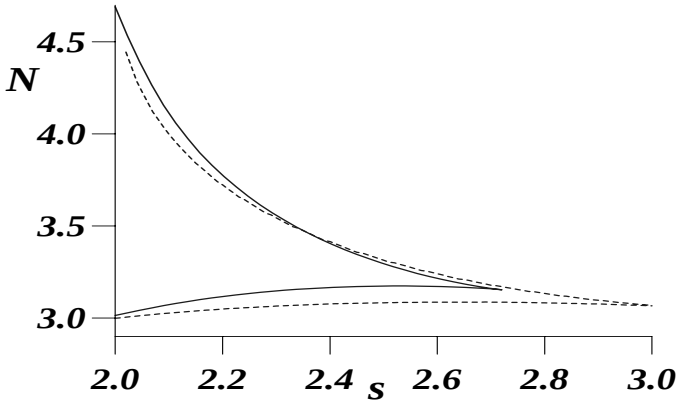

Figure 2: Shows endpoints of the bistability interval for N versus dispersion parameter s. For $s = s_{cr}$ the endpoints coalesce. Analytical dependence (full), $s_{cr} \simeq 2.72$. Numerical dependence (dashed), $s_{cr} \simeq 3.03$.

According to the variational principle we should satisfy the condition $\frac{d\mathcal{H}}{d\alpha} = 0$ which yields

$$N^{\sigma} = 2(\sigma+1)J\,(\tanh(\alpha) \quad F(e^{-\alpha}, s-2) + \tanh^2(\alpha) \quad F(e^{-\alpha}, s-1) \quad)\left(\frac{df_{\sigma}}{d\alpha}\right)^{-1} . \tag{23}$$

As a direct consequence of Eq. (17), frequency Λ can be expressed as

$$\Lambda = -\frac{1}{N}\left(\mathcal{K} + 2\mathcal{V}\right) \tag{24}$$

with $\mathcal{K}$ and $\mathcal{V}$ being defined by Eqs. (19) and (20). Let us discuss first the stationary states of the system for the case $\sigma = 1$.

Figure 1 shows the dependence $N(\Lambda)$ obtained for $\sigma = 1$ from direct numerical solution of Eq. (17). A monotonic function is obtained for $s > s_{cr}$. For $s_{cr} > s > 2$ the dependence becomes non-monotonic (of $\mathcal{N}$-type) with a local maximum and a local minimum. These extrema coalesce at $s = s_{cr} \simeq 3.03$. For $s < 2$ the local maximum disappears. The dependence $N(\Lambda)$ obtained analytically from Eqs. (23) and (24) is in a good qualitative agreement with the

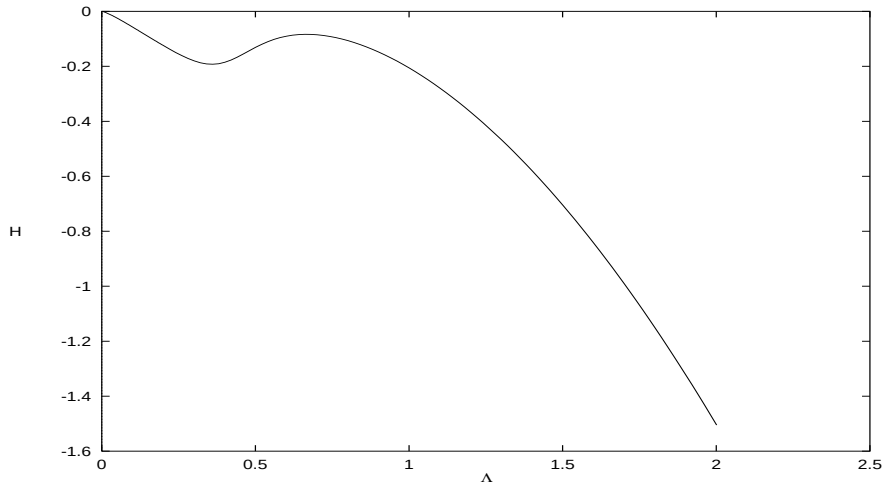

Figure 3: Hamiltonian of the system, $\mathcal{H}$, versus frequency, Λ, numerically from Eq. (17) for $s = 2.5$.

dependence obtained numerically[31]. Thus the main features of all discrete NLS models with dispersive interaction J_{n-m} decreasing faster than $|n-m|^{-s_{cr}}$ coincide qualitatively with the features obtained in the nearest-neighbor approximation where only one on-site stationary state exists for any N. However, for $2 < s < s_{cr}$ three stationary states with frequencies $\Lambda_1(N) < \Lambda_2(N) < \Lambda_3(N)$ there exist for each N in the interval $[N_l(s), N_u(s)]$. In particular, this means that in the case of dipole-dipole interaction ($s = 3$) multiple solutions exist. It is noteworthy that similar results are obtained when the dispersive interaction is in the form of the Kac-Baker potential (6). In this case the bistability takes place for $\beta \leq 1.67$. According to the theorem which was recently proven [33], the necessary and sufficient stability criterion for the stationary states is

$$\frac{dN}{d\Lambda} = \frac{d}{d\Lambda} \sum_n \phi_n^2 > 0 \, . \tag{25}$$

Therefore we can conclude that in the interval $[N_l(s), N_u(s)]$ there are only two linearly stable stationary states ($\Lambda_1(N)$ and $\Lambda_3(N)$). The third state is unstable since $\dfrac{dN}{d\Lambda} < 0$ at $\Lambda = \Lambda_2$.

At the points ($\Lambda(N_l)$ and $\Lambda(N_u)$) the stability condition is violated, since $(\dfrac{\partial N}{\partial \Lambda})_s$ vanishes. Constructing the locus of the end points we obtain the curve

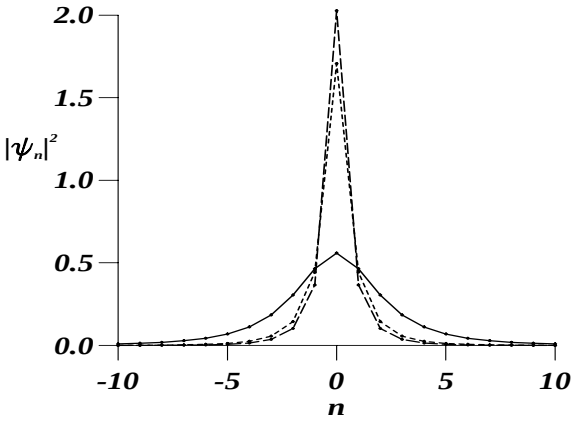

Figure 4: Shapes of the three stationary states for $s = 2.5$ and $N = 3.1$. The stable: $\Lambda = 0.21$ (full), $\Lambda = 0.74$ (long-dashed). The unstable: $\Lambda = 0.57$ (short-dashed).

presented in Fig. 2. This curve bounds the region of bistability. It is analogous to the critical curve in the van der Waals' theory of liquid-vapour phase transition [34]. Thus in the present case we have a similar phase transition like behavior where two phases are the continuum states and the intrinsically localized states, respectively. The analog of temperature is the parameter s. Figure 3 shows the multistability phenomenon in terms of the Hamiltonian $\mathcal{H}$ of the system given by Eqs. (10)–(12) for $\sigma = 1$ and $s = 2.5$. For $s < s_{cr}$ there is an energy interval where for each $\mathcal{H}$ three stationary states with different Λ exist. The observed bistability is very similar to the recently observed one [33,35], where the nearest-neighbor case with an arbitrary degree of nonlinearity σ was studied. The bistability appears in this case for σ above a certain critical value.

Figure 4 shows that the shapes of these solutions differ significantly. The low frequency states are wide and continuum like while the high frequency solutions represent intrinsically localized states with a width of several lattice spacings. It can be obtained [31] that the inverse widths of these two stable states are

$$\alpha_1 \approx \left(\frac{N}{8J}\right)^{1/(s-2)} = \left(\frac{N}{8J}\right)^{\ln \ell/(1-2\ln \ell)}, \quad \alpha_3 \approx \ln\left(\frac{N}{J}\right), \tag{26}$$

where $\ell = \exp(1/s)$ is the characteristic length scale of the dispersive interac-

tion which is defined as a distance at which the interaction decreases twice. It is seen from these expressions that the existence of two so different soliton states for one value of the excitation number, N, is due to the presence of two different length scales in the system: the usual scale of the NLS model which is related to the competition between nonlinearity and dispersion (expressed in terms of the ratio N/J) and the range of the dispersive interaction ℓ.

Now we turn to discus stationary states of the discrete NLS model given by Eq. (17) with arbitrary degree of nonlinearity. The main properties of the system remain unchanged, but the critical value of the dispersion parameter s_{cr} is now a function of σ. The results of analytical consideration confirmed by simulation show that s_{cr} increases with increasing σ. In particular, for $\sigma \geq 1.4$ (the value at which discrete symmetric ground state can be unstable in the nearest-neighbor approximation [33]) the bistability in the nonlinear energy spectrum occurs even for $s \leq 6$.

3 Tails of intrinsically localized states

Investigating the asymptotic behavior of the excitations, it is convenient to rewrite Eq. (17) (we consider here the case $\sigma = 1$) in the form

$$\phi_n \, = \, \sum_m G_{n-m}(\Lambda)\, \phi_n^3 \, , \tag{27}$$

where

$$G_n(\Lambda) = \frac{1}{2\pi} \int\limits_{-\pi}^{\pi} dk \, \frac{\cos(kn)}{\Lambda + \mathcal{L}(k)} \tag{28}$$

is the Green's function with the spectrum function

$$\mathcal{L}(k) = 2 \sum_{n=1}^{\infty} J_n (1 - \cos(kn)) \, . \tag{29}$$

Deriving the asymptotic expressions for the Green's function (28) [31] we obtain that the tails of the intrinsically localized states are given by the expressions

$$\phi_n \to \sqrt{\frac{(\Lambda+1)^3 \zeta(s)}{2\Lambda\zeta(s-2)}} \exp\left(-\sqrt{\frac{2\Lambda\zeta(s)}{\zeta(s-2)}} |n| \right) \, , \quad s > 3 \, , \tag{30}$$

$$\phi_n \to \frac{(\Lambda+1)^{\frac{3}{2}}}{\Lambda^2} |n|^{-s} \, , \quad 2 < s < 3 \, , \tag{31}$$

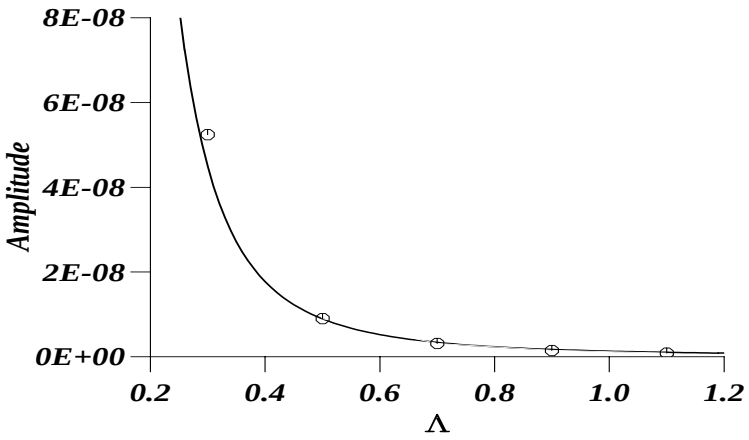

Figure 5: Amplitude in the tail of the stationary state for $s = 2.5$ and $n = 450$. Numerical (circles) and Eq. (31) (full).

for $|n| \to \infty$. Thus we can conclude here that only in the case of the short-range dispersion ($s > 3$) the tails of intrinsically localized states have a usual exponential form. In the systems with long-range dispersive interactions these states have algebraic tails. Figure 5 shows the long-distance behavior of the intrinsically localized states for $s = 2.5$ and different values of the frequency Λ. It is seen that the form of the tails predicted by Eq. (31) is in a good agreement with the results of numerical simulations.

The long-distance behavior of the intrinsically localized states may play an essential role in the thermodynamic properties of the DNA molecule because in systems where the interaction decays algebraically it can be responsible for the appearance of new thermodynamically stable states (for example, quite recently [36] the existence of the Neel order in the ground state of Heisenberg antiferromagnetic chains with algebraic long-range interactions was proven).

4 Switching between bistable states

Having established the existence of bistable stationary states in the nonlocal discrete NLS system, a natural question that arises concerns the role of these states in the full dynamics of the model. In particular, it is of interest to investigate the possibility of switching between the stable states under the influence of external perturbations, and what type of perturbations could be used

to control the switching. Switching of this type is important in the description of nonlinear transport and storage of energy in biomolecules like the DNA, since a mobile continuum-like excitation can provide action at distance while the switching to a discrete, pinned state can facilitate the structural changes of the DNA [16,5]. As it was shown recently [37] the switching will occur if the system is perturbed in a way so that an internal, spatially localized and symmetric mode ('breathing mode') of the stationary state is excited above a threshold value.

To investigate the time evolution of an initially small perturbation $\epsilon_n(0)$ of the stationary state (16) we write

$$\psi_n(\tau) = (\phi_n + \epsilon_n(\tau))\, e^{i\Lambda\,\tau} \tag{32}$$

Decomposing $\epsilon_n(\tau)$ into real and imaginary parts, $\epsilon_n^{(r)}$ and $\epsilon_n^{(i)}$, we obtain from Eq. (14) with $\sigma = 1$ in the linear approximation

$$\frac{d}{d\tau}\begin{pmatrix} \epsilon_n^{(r)} \\ \epsilon_n^{(i)} \end{pmatrix} = \mathcal{M}\begin{pmatrix} \epsilon_n^{(r)} \\ \epsilon_n^{(i)} \end{pmatrix} \equiv \begin{pmatrix} 0 & H^+ \\ -H^- & 0 \end{pmatrix}\begin{pmatrix} \epsilon_n^{(r)} \\ \epsilon_n^{(i)} \end{pmatrix} \tag{33}$$

where, for a system with M sites, H^+ and H^- are $M \times M$ matrices defined by

$$H_{ij}^{\pm} = \left(\Lambda - (2 \mp 1)\phi_i^2 + 2\right)\,\delta_{i,j} - J_{i-j}, \tag{34}$$

with $J_0 = 0$. By definition the stationary solution is linearly stable if the perturbation $\epsilon_n(\tau)$ as calculated from Eq. (33) remains bounded for all times. Linear stability is then equivalent to the matrix $\mathcal{M}$ having no eigenvalues with a positive real part. Changing some parameter (e.g. Λ), a stable state might become unstable. The 'direction' in which an initial perturbation will grow is then determined by the eigenvector corresponding to the eigenvalue of $\mathcal{M}$ with a positive real part. We will in sequel mainly discuss the case when the matrix element of base elastic coupling J_{n-m} decreases exponentially with the distance $|n-m|$ (see Eq. (6)) with the inverse radius of the interaction $\beta = 1$. For such value of β the multistability occurs in the interval $3.23 \leq N \leq 3.78$. It is worth noticing, however, that the scenario of switching described below remains qualitatively unchanged for all values of $\beta \leq 1.67$, and also for the algebraically decaying dispersive coupling with $2 \leq s \leq 3.03$.

The study [37] of the eigenvalue problem for the matrix $\mathcal{M}$ showed the existence of a spatially symmetric internal breathing mode for both the narrow and broad components of the bistable state. Furthermore, the low frequency (broad) component also possesses a spatially antisymmetric translational ("pinning") mode [38]. Since the appearance of a translational mode

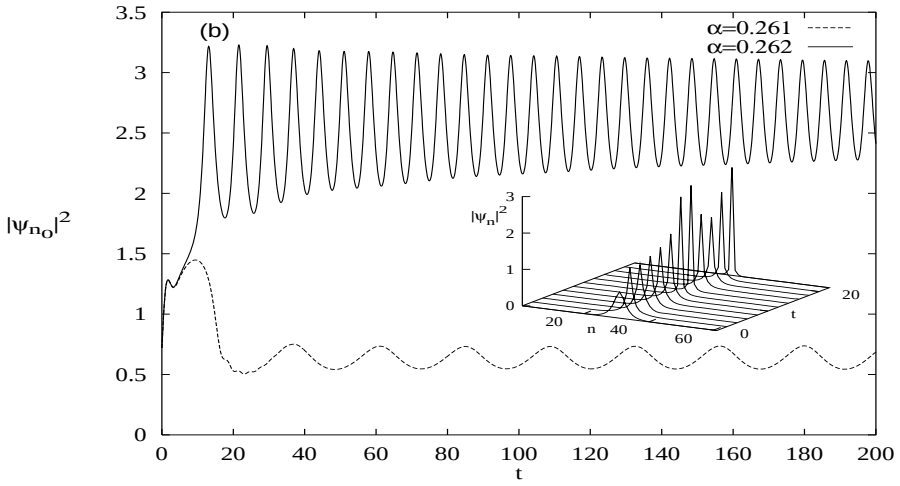

Figure 6: Switching from continuum-like to discrete state for $\beta = 1$. The initial state ϕ_n has the frequency $\Lambda \simeq 0.31$ and $N = 3.6$. The time evolution of $|\psi_{n_0}(\tau)|^2$ when a phase torsion is applied to the center site with $\theta = 0.261$ (lower curve) and $\theta = 0.262$ (upper curve), respectively; inset shows time evolution of $|\psi_n(\tau)|^2$ for $\theta = 0.262$.

implies that the stationary state gains mobility [38], the continuum-like state will have a high mobility.

An illustration of how the presence of an internal breathing mode can affect the dynamics of a slightly perturbed stable stationary state is given in Fig. 6. To excite the breathing mode we apply a spatially symmetric, localized perturbation, which we choose to conserve the number of excitations in order not to change the effective nonlinearity of the system. The simplest choice, which we have used in the simulations shown here, is to kick the central site n_0 of the system at $t = 0$ by adding a parametric force term of the form $\theta\delta_{n,n_0}\delta(\tau)\psi_n(\tau)$ to the left-hand-side of Eq. (14). A possible physical motivation of the appearance of such kind of parametric kick may be the following. It is well known that biomolecules in cells interact with solvent molecules and ions (ligands). At the position where the ligand links to a biomolecule the potential energy of the biomolecule changes. This manifests itself in a local change of the vibration frequency of biomolecular units. In our case it means that the frequency ω of the internal base-pairs oscillations locally changes and the potential energy (4) should be replaced by

$$V = \sum_n \left(V(u_n) + \frac{1}{2}\delta_{nn_0}\theta(\tau)\, u_n^2 \right) \tag{35}$$

where n_0 is the site where the ligand interacts with the biomolecule, θ is a constant which characterizes the energy interaction between the ligand and biomolecule. It may be a function of time because the ligand may attach or detach at different time moments. If we use the rotating wave approximation (8) the NLS model given by Eq. (9) with the additional term in Eq. (12) being

$$\mathcal{V}_{int} = \sum_n \delta_{n\,n_0} \theta(\tau) |\psi_n(\tau)|^2. \tag{36}$$

Assuming that

$$\theta(\tau) = \sum_j \theta_j\, \delta(\tau - \tau_j) \tag{37}$$

we obtain the model where the attachment and detachment of ligands are considered as kicks which occur at the time moments τ_j.

As can be easily shown, this perturbation affects only the site n_0 at $\tau = 0$, and results in a 'twist' of the stationary state at this state with an angle θ, i.e. $\psi_{n_0}(0) = \phi_{n_0}\, e^{i\theta}$. The immediate consequence of this kick is, as can been deduced from the form of Eq. (14), that $\frac{d}{d\tau}\left(|\psi_{n_0}|^2\right)$ will be positive (negative) when $\theta > 0$ ($\theta < 0$). Thus, to obtain switching from the continuum-like state to the discrete state we choose $\theta > 0$, while we choose $\theta < 0$ when investigating switching in the opposite direction. We find that in a large part of the multistability regime there is a well-defined threshold value θ_{th}, such that when the initial phase torsion is smaller than θ_{th}, periodic, slowly decaying 'breather' oscillations around the initial state will occur, while for strong enough kicks (phase torsions larger than θ_{th}) the state switches into the other stable stationary state.

It is worth remarking that the particular choice of perturbation is not important for the qualitative features of the switching, as long as there is a substantial overlap between the perturbation and the internal breathing mode. We believe also that the mechanism for switching described here can be applied for any multistable system where the instability is connected with a breathing mode. For example, we observed [39] a similar switching behavior in the nearest neighbor discrete NLS equation with a higher degree of nonlinearity σ, which is known [33] to exhibit multistability.

5 Conclusion

We have proposed a new nonlocal discrete nonlinear Schrödinger model for the dynamical structure of DNA with long-range (r^{-s} and $e^{-\beta r}$) dispersive interaction. We have shown that there is a multistability in the spectrum of

stationary states of the model with a long-range dispersive interaction $s < s_{cr}$ ($\beta < \beta_{cr}$). There is an energy interval where two stable stationary states exist at each value of the Hamiltonian $\mathcal{H}$. One of these states is a continuum-like soliton and the other one is an intrinsically localized mode. The existence of the bistability phenomenon in the NLS models with a nonlocal dispersion is a result of the competition of two length scales which exist in the system: the scale related to the competition between nonlinearity and dispersion, and the scale related to the dispersion interaction.

We found that the critical value of the dispersion parameter s_{cr} for the on-site stationary state in the case of cubic nonlinearity exceeds 3. This means that the bistable behavior may occur in the case of DNA where the stretching motion of base-pairs is accompanied by a change of their dipole moments.

We have shown that the long-distance behavior of intrinsically localized states in discrete NLS models with a nonlocal dispersion depends drastically on the value of the dispersive parameter s. Only for short-range dispersions the excitation wave functions decay exponentially. In the systems where the matrix element of base elastic coupling depends on the distance slower than $1/r^3$ the nonlinear excitations have algebraic tails. The long-distance behavior may be important for the thermodynamics of DNA since it provides long-range order in one-dimensional systems.

We have shown that a controlled switching between narrow, pinned states and broad, mobile states is possible. Applying a perturbation in the form of parametric kick, we showed that switching occurs beyond some well-defined threshold value of the kick strength.

The particular choice of perturbation is not important for the qualitative features of the switching, as long as there is a substantial overlap between the perturbation and the internal breathing mode. Thus, we believe that the mechanism for switching described here can be applied for any multistable system where the instability is connected with a breathing mode. The switching phenomenon could be important for controlling energy storage and transport in DNA molecules.

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References

1. C. Reiss, in *Nonlinear Excitations in Biomolecules*, Ed.: M. Peyrard (Springer-Verlag Berlin, Heidelberg, Les Editions de Physique Les Ulis, 1995), 29.
2. Lozansky *et al*, in *Stereodynamics of Molecular Systems*, Ed.: R.H. Sarma (Pergamon Press, 1979), 265.
3. K.C. Chou and B. Mao, Biopolymers **27**, 1795 (1988).
4. E.W. Prohovsky, in *Biomolecular Stereodynamics IV*, Eds.: R.H. Sarma and M.H. Sarma (Adenine Guilderland N.Y., 1986), 21.
5. Georghiou *et al*, Biophysical J. **70**, 1909 (1996).
6. S.R. Holbrook and S.H. Kim, J. Mol. Biol. **173**, 361 (1984).
7. Yu.B. Gaididei and A.A. Serikov, Theor. and Math. Phys. **27**, 457 (1976).
8. G.C. Papanicolaou, J. Appl. Math. **21**, 13 (1971).
9. M. Wadati, J. Phys. Soc. Jpn. **38**, 673 (1976).
10. A.J. Sievers and S. Takeno, Phys. Rev. Let. **61**, 970 (1988).
11. R.S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
12. J. Pouget *et al*, Phys. Rev. B **47**,14866 (1993).
13. T. Dauxois and M. Peyrard, Phys. Rev. Let. **70**, 3935 (1993).
14. V. Muto *et al*, Phys. Rev. A **42**, 7452 (1990).
15. P.L. Christiansen *et al*, Phys. Rev. B **55**, 5729 (1997).
16. G. Gaeta *et al*, Riv. N. Chim. **17**, 1 (1994).
17. M. Peyrard and A.R. Bishop, Phys. Rev. Lett. **62**, 2755 (1989).
18. M. Techera, L.L. Daemen, and E.W. Prohofsky, Phy. Rev. A **40**, 6636 (1989).
19. T. Dauxois, M. Peyrard, and A.R. Bishop, Phys. Rev. E **47**, 684 (1993).
20. T. Dauxois, M. Peyrard, and A.R. Bishop, Phys. Rev. E **47**, R44 (1993).
21. U. Dahlborg and A. Rupprecht, Biopolymers **10**, 849 (1971).
22. G. Corongiu and E. Clementi, Biopolymers **20**, 551, (1981).
23. O.M. Braun, Yu.S. Kivshar, and I.I. Zelenskaya, Phys. Rev. B **41**, 7118 (1990).
24. P. Woafo, J.R. Kenne, and T.C. Kofane, J. Phys. Condens. Matter **5**, L123 (1993).
25. G.A. Baker Jr, Phys. Rev. **122**, 1477 (1961).
26. A.M. Kac and B.C. Helfand, J. Math. Phys. **4**, 1078 (1972).
27. L. Vazquez, W.A.B. Evans and G. Rickayzen, Phys. Lett. A **189**, 454 (1994).
28. G.L. Alfimov *et al*, Chaos **3**, 405 (1993).
29. Yu.B. Gaididei *et al*, Phys.Lett. A **222**, 152 (1996); Yu.B. Gaididei *et*

al., Phys. Scr. **T67**, 151 (1996).
30. Yu.B. Gaididei *et al*, Phys. Rev. Lett. **75**, 2240 (1995).
31. Yu.B. Gaididei *et al*, Phys. Rev. E **55**, 6141 (1997).
32. W. Magnus, F. Oberhettinger and R.P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer-Verlag, Berlin, 1966).
33. E.W. Laedke, K.H. Spatschek, and S.K. Turitsyn, Phys. Rev. Lett. **73**, 1055 (1994).
34. L.D. Landau and E.M. Lifshitz, *Statistical Physics* (Pergamon Press, London, 1959).
35. B. Malomed and M.I. Weinstein, Phys. Lett. A **220**, 91 (1996).
36. J.R. Pareira, O. Bolina, and J.F. Perez, J.Phys. A **30**, 1095 (1997).
37. M. Johansson, Yu.B. Gaididei, P.L. Christiansen, and K.Ø. Rasmussen, Phys. Rev. E **57**, 4739 (1998).
38. Ding Chen, S. Aubry, and G. Tsironis, Phys. Rev. Lett. **77**, 4776 (1996).
39. M. Johansson *et al*, Physica D **119**, 115 (1998).